Full wwPDB EM Validation Report ⓘ

Oct 24, 2022 – 06:32 PM EDT

PDB ID	:	7NAQ
EMDB ID	:	EMD-24278
Title	:	Human PA200-20S proteasome complex
Authors	:	Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.
Deposited on	:	2021-06-22
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

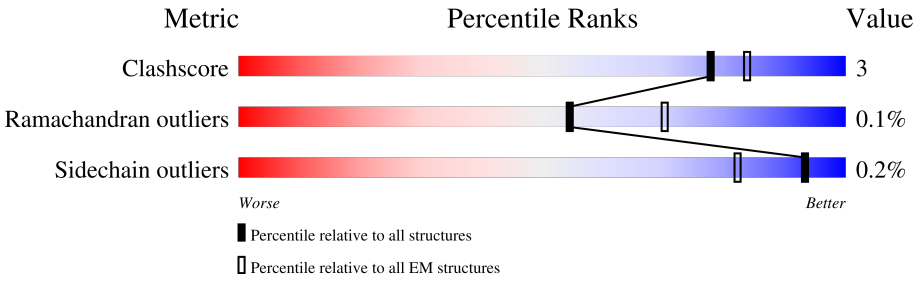
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	88% 5% 7%
1	O	234	90% 9%
2	B	261	86% 13%
2	P	261	89% 7% 5%
3	C	248	86% 5% 9%
3	Q	248	90% 7%
4	D	241	93% 5%
4	R	241	93%

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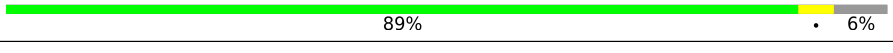
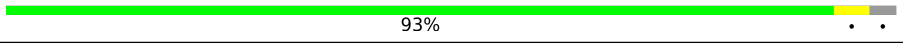
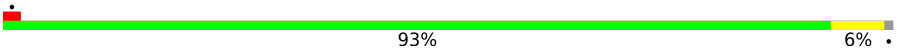
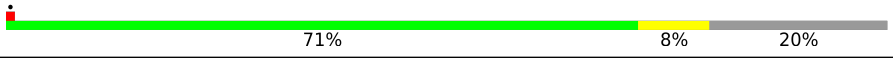
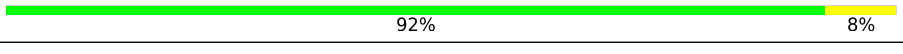
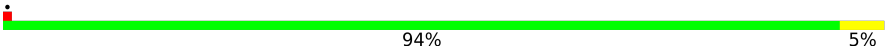
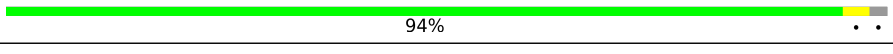
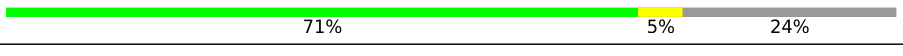
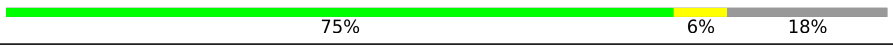
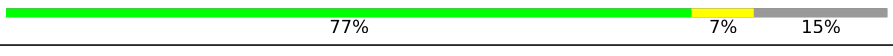
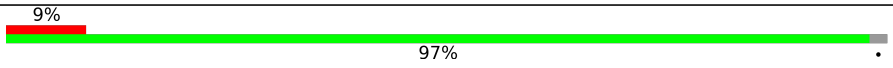
Mol	Chain	Length	Quality of chain
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	c	1843	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 59084 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	217	Total	C	N	O	S	0	0
			1568	1022	281	260	5		
1	O	230	Total	C	N	O	S	0	0
			1677	1093	292	288	4		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	228	Total	C	N	O	S	0	0
			1603	1028	288	283	4		
2	P	249	Total	C	N	O	S	0	0
			1790	1149	318	316	7		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1596	1019	295	280	2		
3	Q	239	Total	C	N	O	S	0	0
			1686	1079	308	294	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	229	Total	C	N	O	S	0	0
			1616	1039	283	285	9		
4	R	235	Total	C	N	O	S	0	0
			1648	1054	289	296	9		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	240	Total	C	N	O	S	0	0
			1806	1147	333	315	11		
5	S	237	Total	C	N	O	S	0	0
			1738	1109	323	299	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	244	Total	C	N	O	S	0	0
			1800	1156	317	319	8		
6	T	240	Total	C	N	O	S	0	0
			1773	1138	313	313	9		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	238	Total	C	N	O	S	0	0
			1742	1123	301	306	12		
7	U	244	Total	C	N	O	S	0	0
			1792	1149	311	321	11		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	0	0
			1598	1017	273	298	10		
8	V	221	Total	C	N	O	S	0	0
			1604	1015	274	305	10		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	0	0
			1548	996	264	270	18		
9	W	204	Total	C	N	O	S	0	0
			1528	982	260	268	18		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1519	984	263	263	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	197	Total	C	N	O	S	0	0
			1514	985	264	257	8		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1518	968	272	269	9		
11	Y	200	Total	C	N	O	S	0	0
			1509	965	269	268	7		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	0	0
			1582	1015	276	281	10		
12	Z	213	Total	C	N	O	S	0	0
			1582	1016	277	279	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1642	1045	290	296	11		
13	a	216	Total	C	N	O	S	0	0
			1635	1043	289	293	10		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1432	914	255	254	9		
14	b	203	Total	C	N	O	S	0	0
			1468	929	259	269	11		

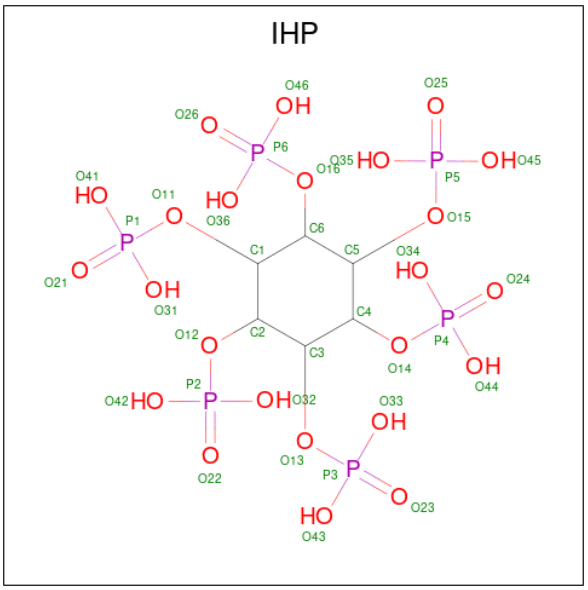
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1799	Total	C	N	O	S	0	0
			13534	8844	2378	2261	51		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	821	ILE	LEU	conflict	UNP Q14997
c	822	LEU	ILE	conflict	UNP Q14997

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



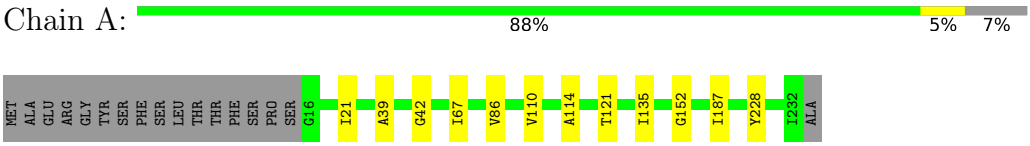
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	c	1	36	6	24	6	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

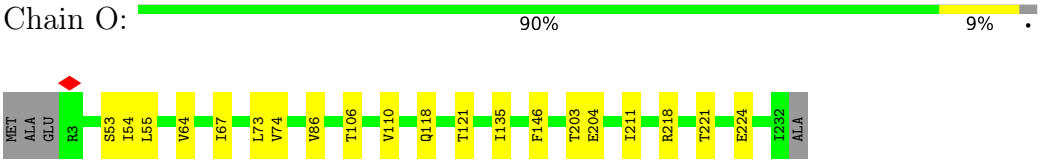
• Molecule 1: Proteasome subunit alpha type-2

Chain A:



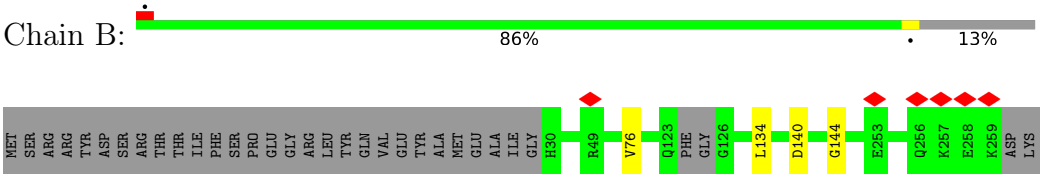
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



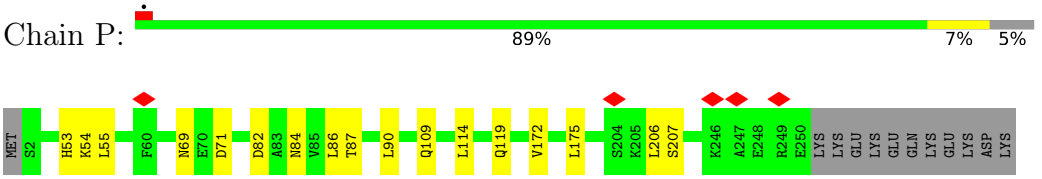
• Molecule 2: Proteasome subunit alpha type-4

Chain B:



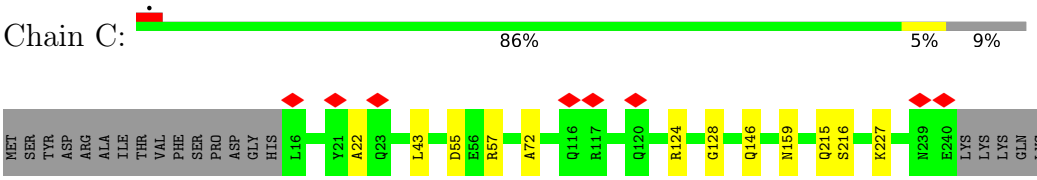
• Molecule 2: Proteasome subunit alpha type-4

Chain P:



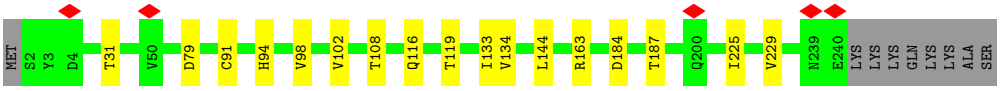
• Molecule 3: Proteasome subunit alpha type-7

Chain C:



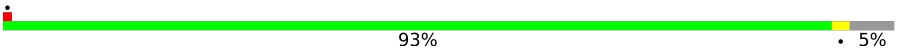
• Molecule 3: Proteasome subunit alpha type-7

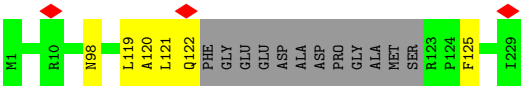
Chain Q:



• Molecule 4: Proteasome subunit alpha type-5

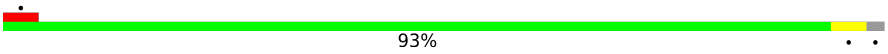
Chain D:

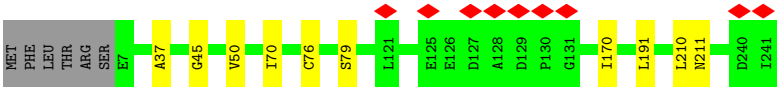




• Molecule 4: Proteasome subunit alpha type-5

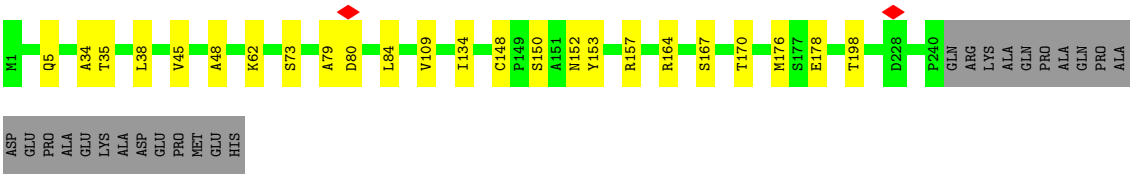
Chain R:





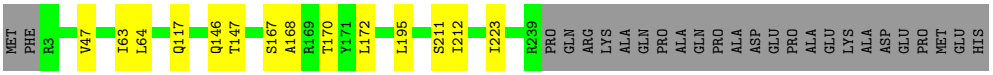
• Molecule 5: Proteasome subunit alpha type-1

Chain E:



• Molecule 5: Proteasome subunit alpha type-1

Chain S:

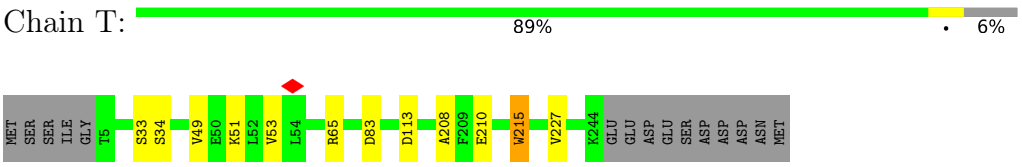


• Molecule 6: Proteasome subunit alpha type-3

Chain F:

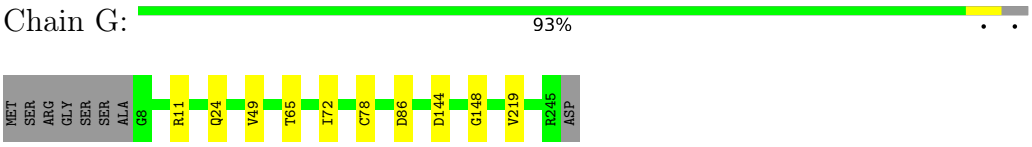
• Molecule 6: Proteasome subunit alpha type-3

Chain T:



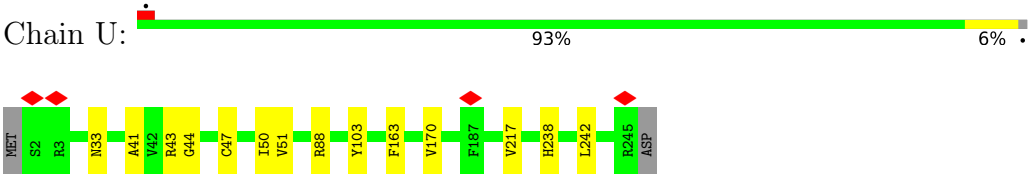
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



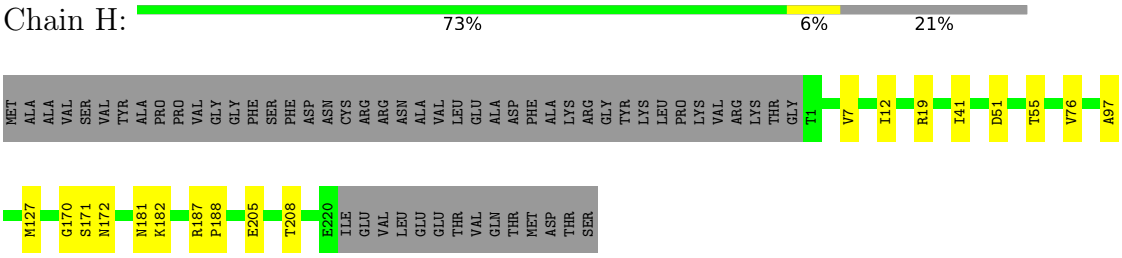
• Molecule 7: Proteasome subunit alpha type-6

Chain U:



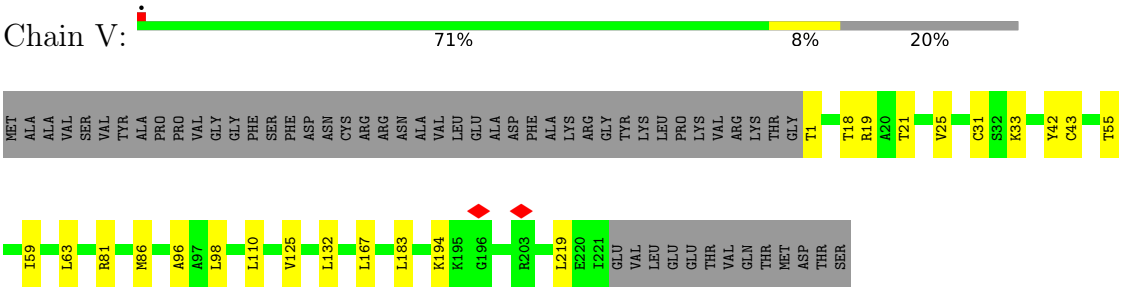
• Molecule 8: Proteasome subunit beta type-7

Chain H:



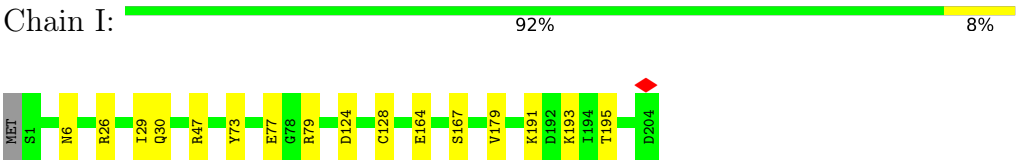
• Molecule 8: Proteasome subunit beta type-7

Chain V:



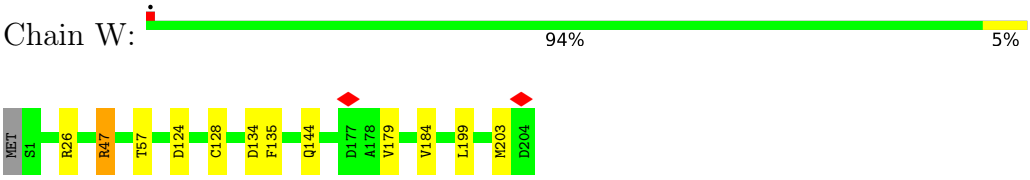
• Molecule 9: Proteasome subunit beta type-3

Chain I:



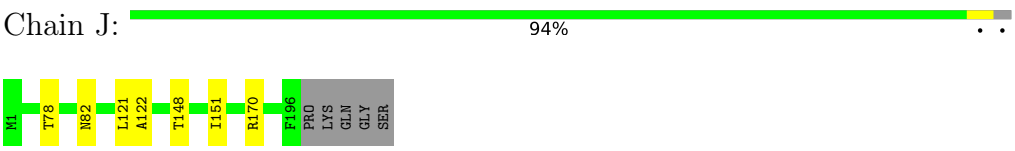
• Molecule 9: Proteasome subunit beta type-3

Chain W:



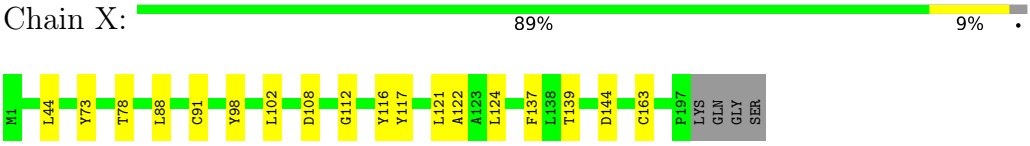
• Molecule 10: Proteasome subunit beta type-2

Chain J:



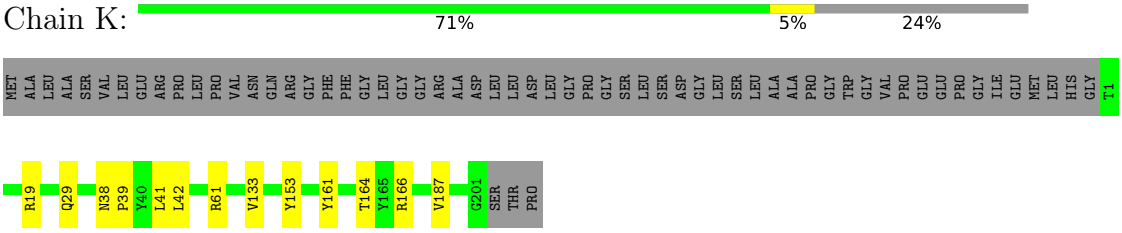
• Molecule 10: Proteasome subunit beta type-2

Chain X:



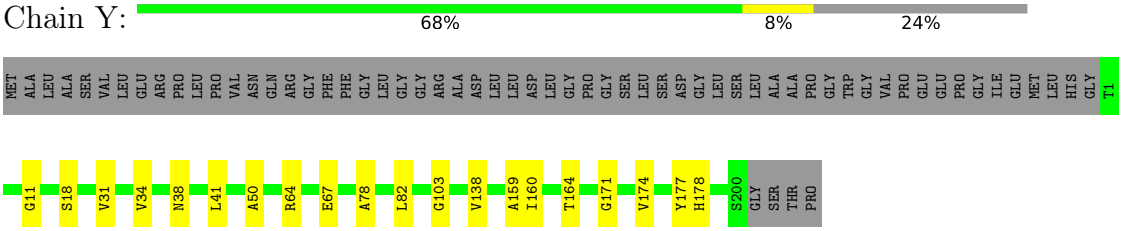
• Molecule 11: Proteasome subunit beta type-5

Chain K:



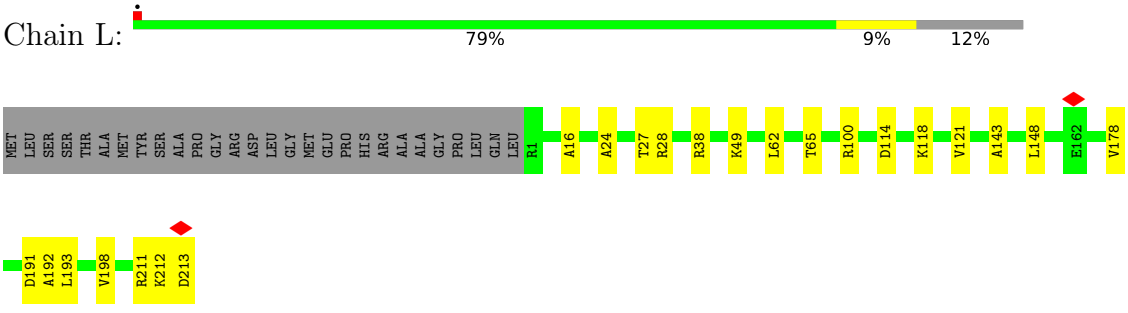
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



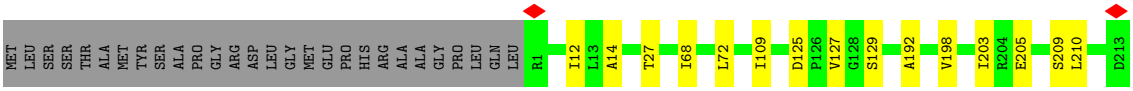
• Molecule 12: Proteasome subunit beta type-1

Chain L:



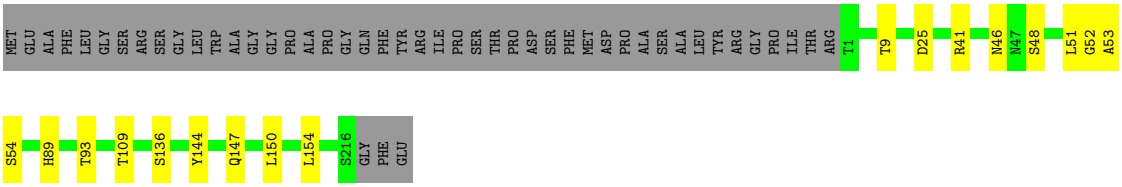
• Molecule 12: Proteasome subunit beta type-1

Chain Z:



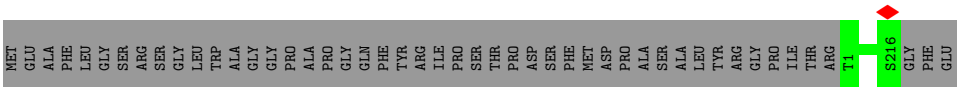
• Molecule 13: Proteasome subunit beta type-4

Chain M:



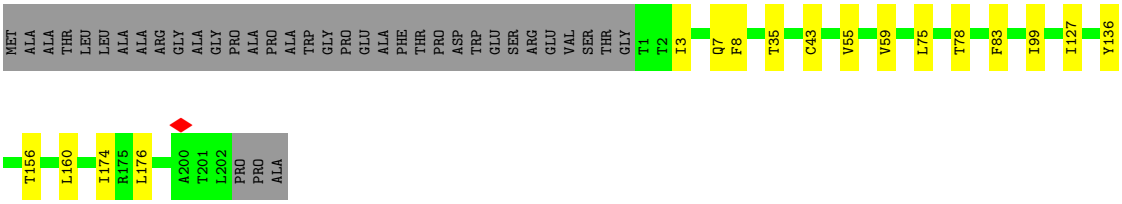
• Molecule 13: Proteasome subunit beta type-4

Chain a:



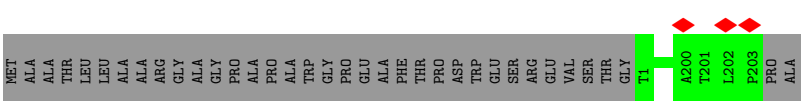
• Molecule 14: Proteasome subunit beta type-6

Chain N:



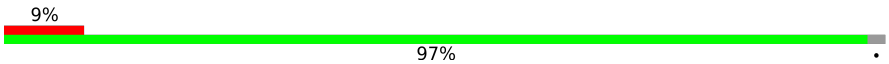
• Molecule 14: Proteasome subunit beta type-6

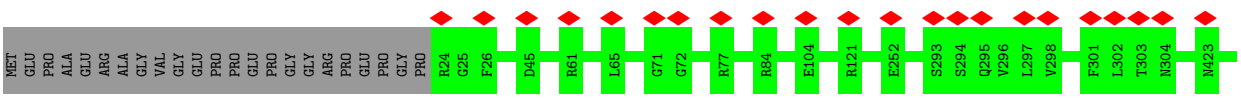
Chain b:

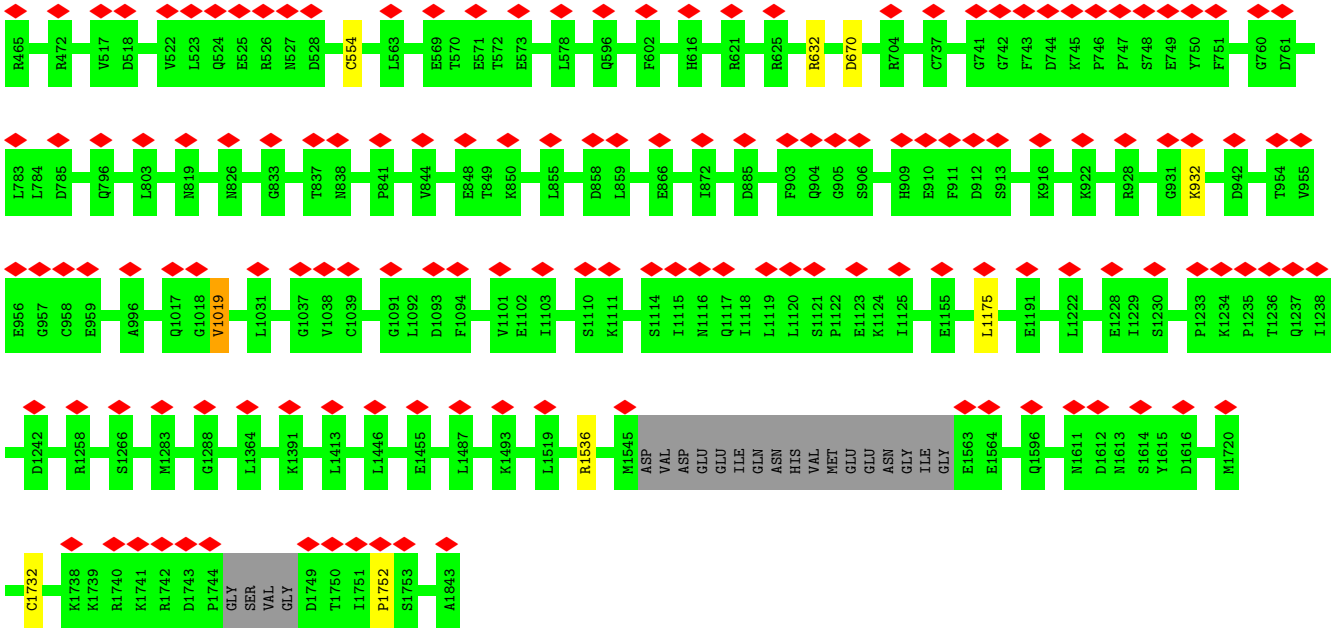


• Molecule 15: Proteasome activator complex subunit 4

Chain c:






R465 R472 V517 D518 V522 L523 Q524 E525 R526 N527 D528 C554 L563 E569 T570 E571 T572 E573 L578 Q596 F602 H616 R621 R625 R632 D670 R704 C737 G741 G742 F743 D744 K745 P746 P747 S748 E749 Y750 F751 G760 D761
L783 L784 D785 Q796 L803 N819 N826 G833 T837 N838 P841 V844 E848 T849 K850 L855 D858 L859 E866 I872 D885 F903 Q904 G905 S906 H909 E910 F911 D912 S913 K916 K922 R928 G931 K932 D942 T954 V955
E956 G957 C958 E959 A996 Q1017 G1018 V1019 L1031 G1037 V1038 C1039 G1091 L1092 D1093 F1094 V1101 E1102 I1103 S1110 K1111 S1114 I1115 N1116 Q1117 I1118 L1119 L1120 S1121 P1122 E1123 K1124 I1125 E1155 L1175 E1191 L1222 E1228 I1229 S1230 P1233 K1234 P1235 T1236 Q1237 I1238
D1242 R1258 S1266 M1283 G1288 L1364 K1391 L1413 L1446 E1455 L1487 K1493 L1519 R1536 M1545 ASP VAL ASP GLU GLU ILE GLN ASN HIS VAL MET GLU GLU ASN GLY ILE GLY E1563 E1564 Q1596 N1611 D1612 N1613 S1614 Y1615 D1616 M1720
C1732 K1738 K1739 R1740 K1741 R1742 D1743 P1744 GLY SER VAL GLY D1749 T1750 I1751 P1752 S1753 A1843

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	24.703	Depositor
Minimum map value	-14.370	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	388.992, 388.992, 388.992	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.56	0/1603	0.56	0/2186
1	O	0.54	0/1716	0.58	0/2342
2	B	0.50	0/1623	0.57	0/2208
2	P	0.47	0/1820	0.58	0/2480
3	C	0.47	0/1616	0.63	0/2201
3	Q	0.45	0/1711	0.58	0/2340
4	D	0.47	0/1641	0.56	0/2234
4	R	0.44	0/1675	0.54	0/2284
5	E	0.52	0/1842	0.61	0/2501
5	S	0.47	0/1772	0.61	0/2414
6	F	0.54	0/1835	0.61	0/2489
6	T	0.51	0/1808	0.56	0/2454
7	G	0.56	0/1775	0.56	0/2420
7	U	0.51	0/1825	0.56	0/2484
8	H	0.58	0/1625	0.64	0/2212
8	V	0.55	0/1630	0.62	0/2217
9	I	0.57	0/1577	0.60	0/2130
9	W	0.58	0/1557	0.59	0/2111
10	J	0.59	0/1551	0.61	1/2106 (0.0%)
10	X	0.61	0/1547	0.60	0/2102
11	K	0.60	0/1549	0.64	0/2098
11	Y	0.57	0/1540	0.62	0/2089
12	L	0.57	0/1612	0.62	1/2180 (0.0%)
12	Z	0.56	0/1612	0.61	0/2180
13	M	0.60	0/1675	0.62	0/2274
13	a	0.61	0/1668	0.63	0/2268
14	N	0.61	0/1458	0.62	0/1985
14	b	0.59	0/1495	0.58	0/2031
15	c	0.38	0/13872	0.56	1/18979 (0.0%)
All	All	0.51	0/60230	0.59	3/81999 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1
15	c	0	4
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	38	ARG	NE-CZ-NH1	5.85	123.23	120.30
10	J	170	ARG	NE-CZ-NH1	5.52	123.06	120.30
15	c	632	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	53	HIS	Peptide
15	c	1019	VAL	Peptide
15	c	1175	LEU	Peptide
15	c	670	ASP	Peptide
15	c	932	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1568	0	1504	7	0
1	O	1677	0	1603	15	0
2	B	1603	0	1515	2	0
2	P	1790	0	1691	11	0
3	C	1596	0	1504	5	0
3	Q	1686	0	1587	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1616	0	1532	5	0
4	R	1648	0	1549	7	0
5	E	1806	0	1749	17	0
5	S	1738	0	1650	9	0
6	F	1800	0	1714	22	0
6	T	1773	0	1676	8	0
7	G	1742	0	1684	7	0
7	U	1792	0	1722	8	0
8	H	1598	0	1567	10	0
8	V	1604	0	1579	16	0
9	I	1548	0	1564	9	0
9	W	1528	0	1504	9	0
10	J	1519	0	1495	3	0
10	X	1514	0	1494	12	0
11	K	1518	0	1458	10	0
11	Y	1509	0	1435	11	0
12	L	1582	0	1547	12	0
12	Z	1582	0	1552	9	0
13	M	1642	0	1593	10	0
13	a	1635	0	1575	0	0
14	N	1432	0	1369	9	0
14	b	1468	0	1417	0	0
15	c	13534	0	13005	0	0
16	c	36	0	6	0	0
All	All	59084	0	56840	232	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:21:THR:OG1	8:V:25:VAL:O	1.99	0.80
5:S:117:GLN:NE2	6:T:83:ASP:OD1	2.15	0.80
14:N:35:THR:OG1	14:N:43:CYS:SG	2.40	0.79
14:N:75:LEU:O	14:N:78:THR:OG1	2.03	0.74
3:C:146:GLN:OE1	3:C:159:ASN:ND2	2.21	0.73
5:E:148:CYS:SG	5:E:150:SER:OG	2.49	0.70
12:L:24:ALA:HB1	12:L:193:LEU:HD11	1.72	0.70
5:E:148:CYS:HG	5:E:150:SER:HG	1.39	0.69
2:P:86:LEU:HD12	2:P:114:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.75	0.68
8:H:205:GLU:O	8:H:208:THR:OG1	2.09	0.68
11:Y:38:ASN:OD1	11:Y:41:LEU:N	2.27	0.68
1:A:110:VAL:HG22	1:A:135:ILE:HD13	1.76	0.66
3:C:55:ASP:OD2	3:C:57:ARG:NH1	2.28	0.66
9:W:26:ARG:NE	9:W:179:VAL:O	2.28	0.66
11:Y:64:ARG:NH1	11:Y:67:GLU:OE2	2.29	0.65
12:Z:125:ASP:OD1	12:Z:129:SER:N	2.29	0.65
14:N:7:GLN:NE2	14:N:8:PHE:O	2.30	0.65
1:O:106:THR:O	1:O:110:VAL:HG23	1.97	0.64
4:R:37:ALA:HB2	4:R:50:VAL:HG23	1.80	0.64
9:W:57:THR:OG1	10:X:121:LEU:O	2.13	0.64
5:S:146:GLN:NE2	5:S:147:THR:O	2.30	0.64
1:O:203:THR:OG1	1:O:204:GLU:OE1	2.16	0.63
12:L:28:ARG:NH2	12:L:191:ASP:OD1	2.32	0.63
13:M:89:HIS:O	13:M:93:THR:HG23	1.98	0.63
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.81	0.62
3:Q:94:HIS:O	3:Q:98:VAL:HG22	1.99	0.62
1:O:110:VAL:HG22	1:O:135:ILE:HD13	1.82	0.62
8:H:171:SER:O	8:H:172:ASN:ND2	2.32	0.62
4:D:119:LEU:O	4:D:122:GLN:N	2.32	0.62
5:S:167:SER:O	5:S:170:THR:OG1	2.18	0.61
9:I:29:ILE:HG22	9:I:30:GLN:H	1.66	0.60
4:D:120:ALA:HB1	4:D:125:PHE:CE2	2.37	0.59
8:H:7:VAL:HG12	8:H:12:ILE:HG22	1.85	0.59
2:P:119:GLN:NE2	3:Q:79:ASP:OD1	2.35	0.59
2:P:90:LEU:HG	2:P:114:LEU:HD13	1.84	0.58
13:M:46:ASN:OD1	13:M:48:SER:N	2.37	0.58
5:E:167:SER:O	5:E:170:THR:OG1	2.17	0.57
13:M:136:SER:OG	13:M:147:GLN:OE1	2.21	0.57
3:Q:31:THR:OG1	3:Q:163:ARG:O	2.13	0.57
9:I:193:LYS:NZ	9:I:195:THR:OG1	2.38	0.57
3:C:215:GLN:NE2	3:C:216:SER:O	2.37	0.57
7:U:43:ARG:NH1	7:U:163:PHE:O	2.38	0.56
6:F:159:GLY:H	7:G:65:THR:HG21	1.71	0.56
3:Q:116:GLN:O	3:Q:119:THR:OG1	2.21	0.56
5:E:35:THR:HG21	5:E:73:SER:CB	2.36	0.56
13:M:144:TYR:HB3	8:V:132:LEU:HD12	1.88	0.56
3:Q:94:HIS:ND1	3:Q:102:VAL:HG22	2.20	0.56
6:F:69:VAL:HG23	6:F:73:VAL:HG13	1.87	0.56
8:H:181:ASN:OD1	8:H:182:LYS:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:51:VAL:HG12	7:U:217:VAL:HG22	1.89	0.55
5:E:157:ARG:NH2	5:E:176:MET:SD	2.81	0.54
10:J:78:THR:O	10:J:82:ASN:ND2	2.37	0.54
6:F:215:TRP:CZ3	6:F:227:VAL:HG13	2.43	0.54
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.37	0.54
10:X:91:CYS:HG	10:X:98:TYR:HE2	1.54	0.54
5:E:34:ALA:O	5:E:62:LYS:NZ	2.41	0.54
6:F:87:LEU:HD13	6:F:135:PHE:CE1	2.43	0.53
6:T:51:LYS:O	6:T:210:GLU:N	2.41	0.53
10:X:44:LEU:HD11	10:X:102:LEU:HD12	1.90	0.53
6:F:189:ILE:O	6:F:193:VAL:HG23	2.07	0.53
4:D:121:LEU:HD22	5:E:79:ALA:HB1	1.90	0.53
5:E:157:ARG:NH2	6:F:56:LYS:O	2.41	0.53
8:V:18:THR:OG1	8:V:31:CYS:N	2.41	0.53
11:Y:160:ILE:HG21	11:Y:174:VAL:HG23	1.90	0.53
13:M:41:ARG:NH1	13:M:53:ALA:O	2.42	0.53
12:L:62:LEU:O	12:L:65:THR:OG1	2.25	0.52
10:X:139:THR:HG23	10:X:163:CYS:HB3	1.92	0.52
5:S:63:ILE:HG21	5:S:223:ILE:HD13	1.91	0.52
7:G:49:VAL:HG12	7:G:219:VAL:HG12	1.92	0.52
3:Q:184:ASP:O	3:Q:187:THR:OG1	2.24	0.52
4:D:98:ASN:OD1	11:K:61:ARG:NH2	2.41	0.51
8:V:19:ARG:NH2	8:V:167:LEU:O	2.44	0.51
6:F:69:VAL:CG2	6:F:73:VAL:HG13	2.41	0.51
3:Q:108:THR:HG22	3:Q:133:ILE:HD13	1.93	0.51
1:O:204:GLU:OE1	1:O:204:GLU:N	2.42	0.51
9:W:134:ASP:OD1	9:W:135:PHE:N	2.43	0.51
8:V:43:CYS:SG	8:V:98:LEU:HD12	2.51	0.50
12:L:143:ALA:HB1	9:W:144:GLN:OE1	2.11	0.50
12:L:148:LEU:HD23	12:L:178:VAL:HG22	1.92	0.50
14:N:3:ILE:HD12	14:N:99:ILE:HD12	1.94	0.50
9:I:26:ARG:NH2	9:I:179:VAL:O	2.43	0.50
6:F:6:GLY:HA2	6:F:9:LEU:HD13	1.94	0.50
12:L:49:LYS:O	12:L:198:VAL:HG11	2.10	0.50
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.11	0.50
11:Y:164:THR:HG22	11:Y:171:GLY:N	2.27	0.50
5:E:152:ASN:OD1	5:E:153:TYR:N	2.45	0.50
14:N:59:VAL:HG11	14:N:83:PHE:CZ	2.47	0.50
6:F:34:SER:CB	6:F:52:LEU:HD23	2.42	0.49
12:Z:12:ILE:HD12	12:Z:109:ILE:HD12	1.94	0.49
6:T:215:TRP:CE3	6:T:227:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:34:VAL:HG11	11:Y:177:TYR:CE1	2.47	0.49
12:Z:27:THR:OG1	12:Z:192:ALA:HB3	2.12	0.49
6:F:186:CYS:O	6:F:190:VAL:HG23	2.12	0.49
9:W:203:MET:SD	9:W:203:MET:N	2.85	0.49
11:K:41:LEU:O	11:K:42:LEU:HD22	2.13	0.49
13:M:144:TYR:CB	8:V:132:LEU:HD12	2.43	0.49
14:N:55:VAL:O	14:N:59:VAL:HG12	2.13	0.49
1:O:67:ILE:HD11	1:O:73:LEU:CD1	2.43	0.48
7:U:238:HIS:O	7:U:242:LEU:HD23	2.14	0.48
13:M:9:THR:OG1	13:M:25:ASP:OD2	2.28	0.48
7:U:103:TYR:O	8:V:81:ARG:NH2	2.47	0.48
2:P:82:ASP:O	2:P:86:LEU:HD23	2.14	0.48
12:Z:198:VAL:HG22	12:Z:203:ILE:HD12	1.96	0.48
9:I:124:ASP:OD1	9:I:128:CYS:N	2.44	0.48
1:O:211:ILE:HD11	1:O:218:ARG:NH2	2.29	0.48
6:F:36:ALA:HB1	6:F:49:VAL:HG12	1.96	0.47
6:F:120:HIS:NE2	7:G:86:ASP:OD1	2.48	0.47
12:L:27:THR:OG1	12:L:192:ALA:HB3	2.13	0.47
9:I:6:ASN:O	9:I:26:ARG:NH2	2.46	0.47
1:O:221:THR:HG23	1:O:224:GLU:H	1.78	0.47
2:P:54:LYS:O	2:P:55:LEU:HD22	2.14	0.47
7:G:144:ASP:O	7:G:148:GLY:N	2.44	0.47
6:F:213:LEU:HB3	6:F:227:VAL:HG21	1.96	0.47
1:A:21:ILE:HD11	1:A:121:THR:OG1	2.14	0.46
8:V:219:LEU:HD13	9:W:47:ARG:HE	1.79	0.46
11:K:153:TYR:CE2	11:K:187:VAL:HG21	2.50	0.46
1:O:64:VAL:HG22	1:O:74:VAL:HG22	1.98	0.46
3:Q:91:CYS:HA	3:Q:102:VAL:HG21	1.97	0.46
5:S:211:SER:HB3	5:S:223:ILE:HD11	1.98	0.46
8:V:59:ILE:O	8:V:63:LEU:HD23	2.15	0.46
6:F:36:ALA:CB	6:F:49:VAL:HG12	2.46	0.46
6:F:215:TRP:CE3	6:F:227:VAL:HG22	2.50	0.46
6:T:53:VAL:HG12	6:T:208:ALA:O	2.16	0.46
14:N:156:THR:O	14:N:160:LEU:HD23	2.16	0.46
5:E:178:GLU:OE1	5:E:178:GLU:N	2.49	0.46
5:E:80:ASP:O	5:E:84:LEU:HD23	2.16	0.46
6:F:124:LEU:HD23	6:F:124:LEU:H	1.81	0.46
4:R:79:SER:HB3	4:R:170:ILE:HD12	1.97	0.46
1:O:110:VAL:HG22	1:O:135:ILE:CD1	2.46	0.45
12:Z:68:ILE:O	12:Z:72:LEU:HD23	2.16	0.45
11:K:166:ARG:NE	10:X:144:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:GLN:O	1:O:121:THR:OG1	2.29	0.45
12:L:211:ARG:NH1	12:L:213:ASP:OD2	2.50	0.45
1:O:211:ILE:HD11	1:O:218:ARG:CZ	2.46	0.45
5:S:63:ILE:C	5:S:64:LEU:HD22	2.37	0.45
8:H:51:ASP:O	8:H:55:THR:HG22	2.16	0.45
10:X:108:ASP:O	10:X:112:GLY:N	2.48	0.45
1:A:110:VAL:HG22	1:A:135:ILE:CD1	2.44	0.45
4:R:70:ILE:HD11	4:R:76:CYS:SG	2.57	0.45
3:Q:225:ILE:O	3:Q:229:VAL:HG13	2.17	0.45
1:A:114:ALA:HB1	1:A:152:GLY:O	2.17	0.45
2:B:76:VAL:HG22	2:B:134:LEU:HD22	1.98	0.45
8:H:19:ARG:HE	8:H:170:GLY:HA3	1.82	0.45
2:P:109:GLN:NE2	10:X:73:TYR:OH	2.50	0.45
5:S:168:ALA:O	5:S:172:LEU:HD23	2.17	0.45
9:W:124:ASP:OD1	9:W:128:CYS:N	2.42	0.45
6:F:70:ASP:HB3	6:F:73:VAL:HG12	1.99	0.44
8:V:110:LEU:HD21	8:V:125:VAL:HG22	2.00	0.44
13:M:150:LEU:O	13:M:154:LEU:HD23	2.17	0.44
14:N:127:ILE:HD11	14:N:136:TYR:CD1	2.53	0.44
1:O:53:SER:O	1:O:55:LEU:N	2.51	0.44
1:O:110:VAL:HG21	1:O:146:PHE:CD2	2.52	0.44
12:Z:205:GLU:N	12:Z:205:GLU:OE1	2.50	0.44
6:F:159:GLY:N	7:G:65:THR:HG21	2.33	0.44
2:P:206:LEU:HD23	2:P:207:SER:N	2.33	0.44
6:T:113:ASP:OD2	7:U:88:ARG:NH2	2.46	0.44
12:Z:14:ALA:CB	12:Z:109:ILE:HG21	2.48	0.44
6:F:39:ILE:HD12	6:F:193:VAL:HG22	2.00	0.44
13:M:51:LEU:HD12	13:M:52:GLY:N	2.32	0.44
5:E:35:THR:OG1	5:E:62:LYS:NZ	2.35	0.43
4:R:45:GLY:CA	4:R:191:LEU:HD21	2.47	0.43
11:K:133:VAL:HG21	10:X:137:PHE:HB3	2.00	0.43
7:U:44:GLY:N	7:U:47:CYS:O	2.46	0.43
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.00	0.43
12:L:16:ALA:HB2	12:L:121:VAL:HG23	2.00	0.43
8:V:55:THR:HG23	8:V:86:MET:CE	2.49	0.43
10:X:78:THR:HG22	10:X:116:TYR:OH	2.18	0.43
14:N:174:ILE:HG22	14:N:176:LEU:CD2	2.48	0.43
7:U:41:ALA:HB2	7:U:50:ILE:HD13	2.01	0.43
2:B:140:ASP:O	2:B:144:GLY:N	2.46	0.43
12:L:28:ARG:NH2	12:L:212:LYS:O	2.52	0.43
11:K:153:TYR:CZ	11:K:187:VAL:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:117:TYR:O	10:X:124:LEU:HD12	2.19	0.43
1:A:187:ILE:HD13	1:A:228:TYR:CZ	2.54	0.43
2:P:172:VAL:HA	2:P:175:LEU:HD12	2.00	0.42
4:R:210:LEU:HD23	4:R:211:ASN:N	2.33	0.42
8:H:97:ALA:HB1	8:H:127:MET:CE	2.49	0.42
9:I:164:GLU:O	9:I:167:SER:OG	2.30	0.42
11:Y:50:ALA:HB2	12:Z:127:VAL:HG13	2.01	0.42
12:L:28:ARG:NE	12:L:191:ASP:OD2	2.47	0.42
3:Q:134:VAL:HG12	3:Q:144:LEU:HA	2.02	0.42
6:F:215:TRP:HZ3	6:F:227:VAL:HG13	1.83	0.42
7:G:72:ILE:HD11	7:G:78:CYS:SG	2.59	0.42
5:E:5:GLN:HG3	6:F:9:LEU:HD11	2.01	0.42
4:R:79:SER:CB	4:R:170:ILE:HD12	2.50	0.42
1:O:73:LEU:HD12	1:O:86:VAL:HG22	2.01	0.42
11:K:161:TYR:O	11:K:164:THR:OG1	2.31	0.42
4:R:37:ALA:HB3	4:R:170:ILE:HD11	2.01	0.42
6:T:33:SER:OG	6:T:34:SER:N	2.52	0.42
2:P:84:ASN:O	2:P:87:THR:OG1	2.34	0.42
2:P:86:LEU:CD1	2:P:114:LEU:HD11	2.45	0.42
10:J:148:THR:H	10:J:151:ILE:HD11	1.84	0.41
8:V:219:LEU:HD13	9:W:47:ARG:NE	2.35	0.41
1:O:67:ILE:HD11	1:O:73:LEU:HD12	2.02	0.41
6:T:49:VAL:HG11	6:T:65:ARG:HB2	2.02	0.41
10:X:44:LEU:CD1	10:X:102:LEU:HD12	2.50	0.41
5:E:35:THR:HG23	5:E:48:ALA:HB2	2.01	0.41
11:K:19:ARG:HE	11:K:29:GLN:HE22	1.68	0.41
6:T:215:TRP:HE3	6:T:227:VAL:HG22	1.85	0.41
8:V:1:THR:HG23	8:V:33:LYS:NZ	2.35	0.41
10:J:121:LEU:O	10:J:122:ALA:HB3	2.21	0.41
1:A:39:ALA:HB3	1:A:42:GLY:O	2.21	0.41
5:E:109:VAL:HG12	5:E:134:ILE:HD13	2.03	0.41
8:V:96:ALA:HB1	8:V:98:LEU:HD21	2.02	0.41
11:Y:18:SER:O	11:Y:31:VAL:HG12	2.21	0.41
11:Y:41:LEU:HD13	11:Y:103:GLY:HA3	2.03	0.41
10:X:88:LEU:HG	10:X:122:ALA:HB2	2.01	0.41
11:Y:138:VAL:HG11	11:Y:159:ALA:HA	2.02	0.41
3:C:22:ALA:HB1	3:C:128:GLY:HA2	2.02	0.41
11:K:38:ASN:OD1	11:K:41:LEU:N	2.54	0.41
8:V:42:TYR:CE1	8:V:183:LEU:HD11	2.56	0.41
5:E:38:LEU:HD23	5:E:45:VAL:HG23	2.03	0.41
8:H:187:ARG:HB3	8:H:188:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:47:ARG:NH2	9:I:191:LYS:O	2.53	0.41
2:P:69:ASN:OD1	2:P:71:ASP:N	2.47	0.41
8:V:1:THR:HG23	8:V:33:LYS:HZ2	1.86	0.41
9:I:77:GLU:O	9:I:79:ARG:N	2.53	0.41
12:L:114:ASP:OD1	12:L:118:LYS:N	2.54	0.41
13:M:54:SER:O	13:M:109:THR:N	2.49	0.41
11:Y:78:ALA:O	11:Y:82:LEU:HD13	2.21	0.41
5:S:212:ILE:O	5:S:223:ILE:HD12	2.20	0.40
5:E:164:ARG:O	5:E:198:THR:HG22	2.22	0.40
7:U:33:ASN:OD1	7:U:170:VAL:HG12	2.22	0.40
11:Y:11:GLY:HA3	11:Y:178:HIS:HE2	1.85	0.40
3:C:43:LEU:HD11	3:C:72:ALA:HB2	2.03	0.40
4:D:120:ALA:HB1	4:D:125:PHE:CD2	2.57	0.40
9:W:184:VAL:HG13	9:W:199:LEU:HD12	2.03	0.40
1:A:67:ILE:CD1	1:A:86:VAL:HG23	2.51	0.40
7:G:11:ARG:O	7:G:24:GLN:NE2	2.49	0.40
9:I:73:TYR:OH	9:I:79:ARG:NH2	2.55	0.40
12:Z:209:SER:C	12:Z:210:LEU:HD12	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/234 (92%)	214 (100%)	1 (0%)	0	100	100
1	O	228/234 (97%)	225 (99%)	2 (1%)	1 (0%)	34	69
2	B	224/261 (86%)	222 (99%)	2 (1%)	0	100	100
2	P	247/261 (95%)	241 (98%)	6 (2%)	0	100	100
3	C	221/248 (89%)	211 (96%)	10 (4%)	0	100	100
3	Q	235/248 (95%)	233 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	224/241 (93%)	222 (99%)	2 (1%)	0	100	100
4	R	233/241 (97%)	232 (100%)	1 (0%)	0	100	100
5	E	238/263 (90%)	233 (98%)	5 (2%)	0	100	100
5	S	235/263 (89%)	234 (100%)	1 (0%)	0	100	100
6	F	242/255 (95%)	237 (98%)	4 (2%)	1 (0%)	34	69
6	T	238/255 (93%)	238 (100%)	0	0	100	100
7	G	236/246 (96%)	232 (98%)	4 (2%)	0	100	100
7	U	242/246 (98%)	242 (100%)	0	0	100	100
8	H	218/277 (79%)	214 (98%)	4 (2%)	0	100	100
8	V	219/277 (79%)	215 (98%)	4 (2%)	0	100	100
9	I	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	191 (98%)	4 (2%)	0	100	100
11	K	199/263 (76%)	198 (100%)	1 (0%)	0	100	100
11	Y	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
12	L	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
12	Z	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
13	M	214/264 (81%)	211 (99%)	3 (1%)	0	100	100
13	a	214/264 (81%)	212 (99%)	2 (1%)	0	100	100
14	N	200/239 (84%)	199 (100%)	1 (0%)	0	100	100
14	b	201/239 (84%)	201 (100%)	0	0	100	100
15	c	1793/1843 (97%)	1743 (97%)	48 (3%)	2 (0%)	51	83
All	All	7929/8719 (91%)	7792 (98%)	133 (2%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	54	ILE
15	c	1019	VAL
15	c	1752	PRO
6	F	227	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/191 (70%)	134 (100%)	0	100 100
1	O	148/191 (78%)	148 (100%)	0	100 100
2	B	133/221 (60%)	133 (100%)	0	100 100
2	P	156/221 (71%)	156 (100%)	0	100 100
3	C	134/211 (64%)	132 (98%)	2 (2%)	65 85
3	Q	146/211 (69%)	146 (100%)	0	100 100
4	D	145/203 (71%)	145 (100%)	0	100 100
4	R	147/203 (72%)	147 (100%)	0	100 100
5	E	175/224 (78%)	175 (100%)	0	100 100
5	S	158/224 (70%)	158 (100%)	0	100 100
6	F	163/212 (77%)	162 (99%)	1 (1%)	86 94
6	T	160/212 (76%)	159 (99%)	1 (1%)	86 94
7	G	165/210 (79%)	165 (100%)	0	100 100
7	U	169/210 (80%)	169 (100%)	0	100 100
8	H	158/228 (69%)	158 (100%)	0	100 100
8	V	163/228 (72%)	162 (99%)	1 (1%)	86 94
9	I	158/174 (91%)	158 (100%)	0	100 100
9	W	151/174 (87%)	150 (99%)	1 (1%)	84 94
10	J	148/171 (86%)	148 (100%)	0	100 100
10	X	145/171 (85%)	145 (100%)	0	100 100
11	K	137/202 (68%)	137 (100%)	0	100 100
11	Y	133/202 (66%)	133 (100%)	0	100 100
12	L	153/199 (77%)	152 (99%)	1 (1%)	84 94
12	Z	153/199 (77%)	153 (100%)	0	100 100
13	M	160/215 (74%)	160 (100%)	0	100 100
13	a	156/215 (73%)	156 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	126/181 (70%)	126 (100%)	0	100 100
14	b	139/181 (77%)	139 (100%)	0	100 100
15	c	1291/1673 (77%)	1288 (100%)	3 (0%)	93 98
All	All	5504/7357 (75%)	5494 (100%)	10 (0%)	93 98

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	124	ARG
3	C	227	LYS
6	F	179	LEU
12	L	100	ARG
6	T	215	TRP
8	V	194	LYS
9	W	47	ARG
15	c	554	CYS
15	c	1536	ARG
15	c	1732	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
3	C	94	HIS
3	C	215	GLN
6	F	63	ASN
10	J	63	ASN
10	J	186	ASN
11	K	29	GLN
11	K	191	ASN
12	L	152	GLN
13	M	108	ASN
14	N	7	GLN
2	P	109	GLN
2	P	167	ASN
5	S	8	ASN
6	T	63	ASN
6	T	97	ASN
9	W	39	GLN
9	W	172	ASN

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Mol	Chain	Res	Type
10	X	61	GLN
12	Z	152	GLN
12	Z	157	ASN
15	c	607	GLN
15	c	877	ASN
15	c	984	ASN
15	c	1145	ASN
15	c	1496	GLN
15	c	1714	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	IHP	c	1901	-	36,36,36	0.83	0	54,60,60	1.30	5 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	IHP	c	1901	-	-	4/30/54/54	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	1901	IHP	C6-C5-C4	3.37	117.79	110.41
16	c	1901	IHP	C5-C6-C1	3.18	117.37	110.41
16	c	1901	IHP	O15-C5-C4	2.50	114.57	108.69
16	c	1901	IHP	C6-C1-C2	2.29	115.42	110.41
16	c	1901	IHP	O16-C6-C5	2.05	113.52	108.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

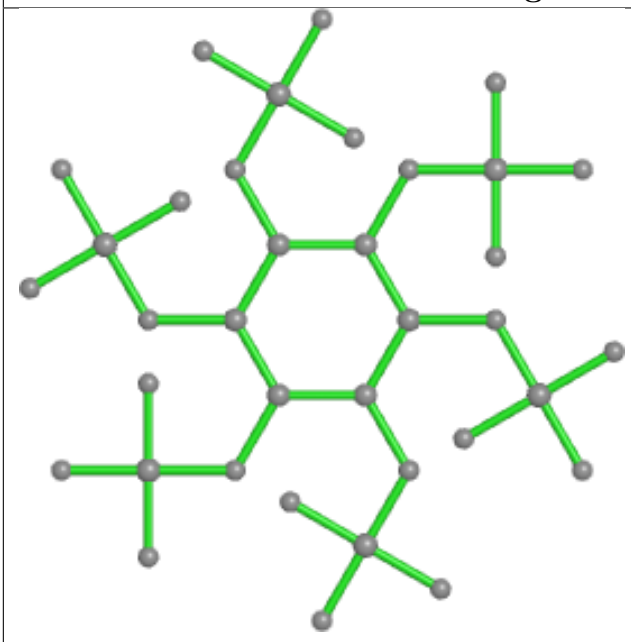
Mol	Chain	Res	Type	Atoms
16	c	1901	IHP	C4-C5-O15-P5
16	c	1901	IHP	C6-C5-O15-P5
16	c	1901	IHP	C5-O15-P5-O25
16	c	1901	IHP	C1-O11-P1-O31

There are no ring outliers.

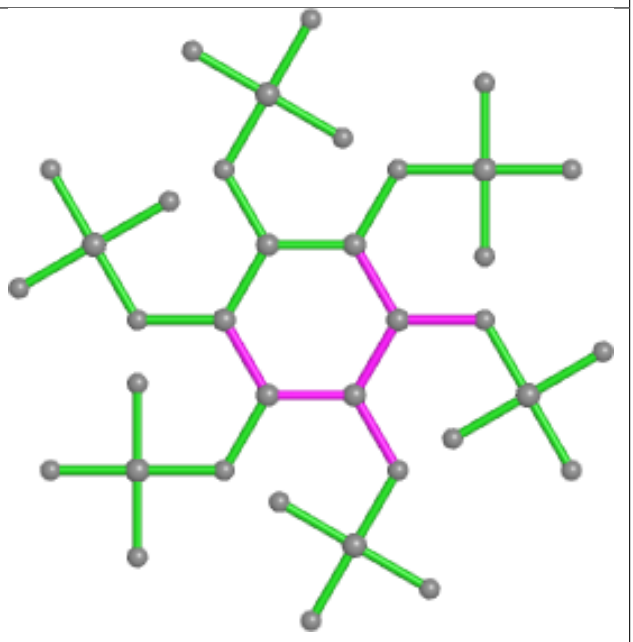
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

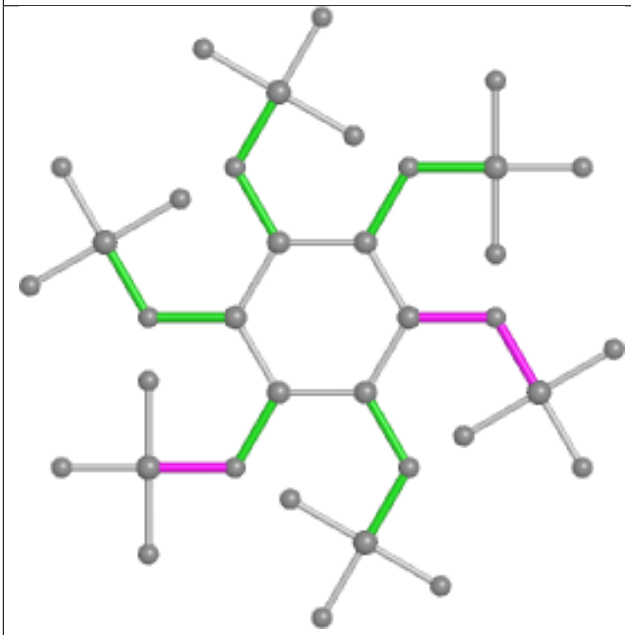
Ligand IHP c 1901



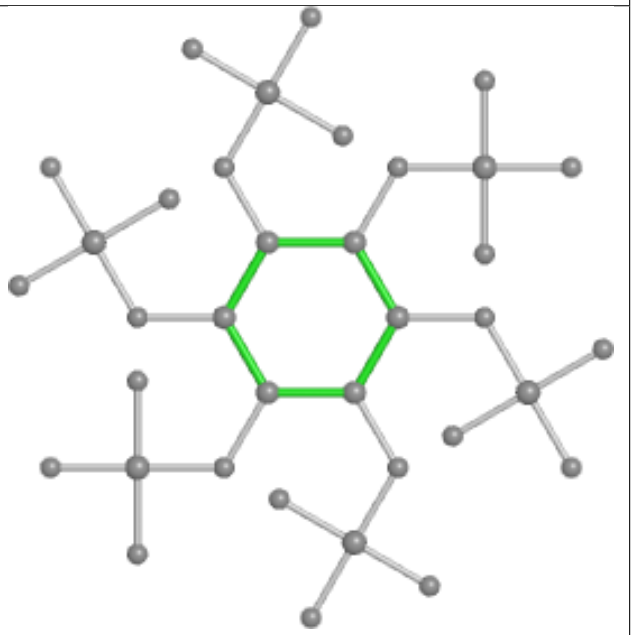
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1
3	Q	1
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	116:GLN	C	117:ARG	N	3.61
1	Q	199:VAL	C	200:GLN	N	3.56
1	D	121:LEU	C	122:GLN	N	3.06

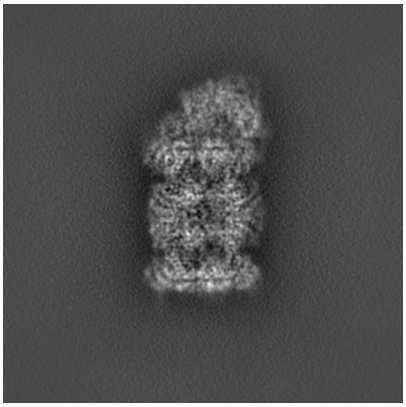
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24278. These allow visual inspection of the internal detail of the map and identification of artifacts.

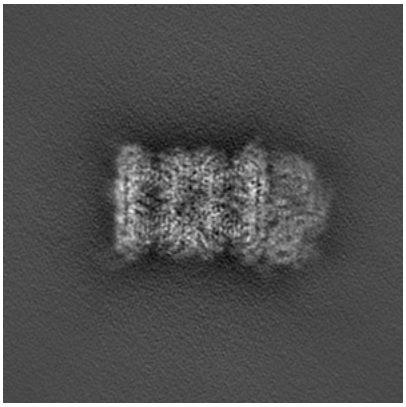
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

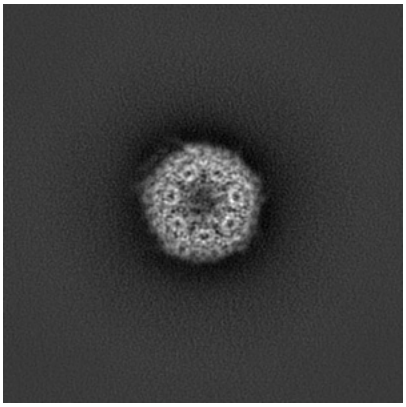
6.1.1 Primary map



X



Y

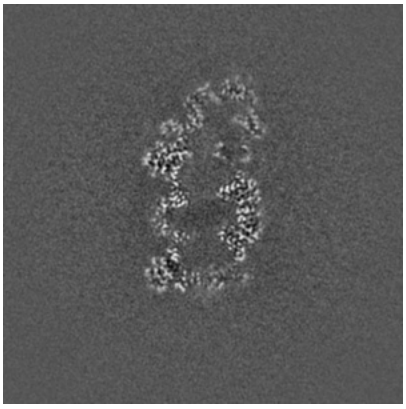


Z

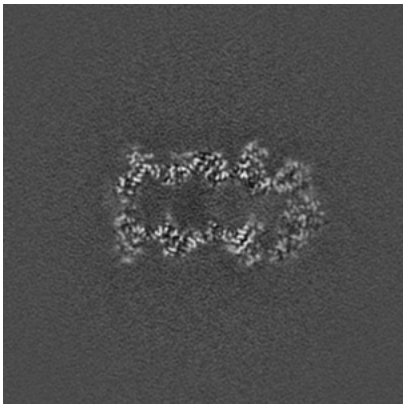
The images above show the map projected in three orthogonal directions.

6.2 Central slices

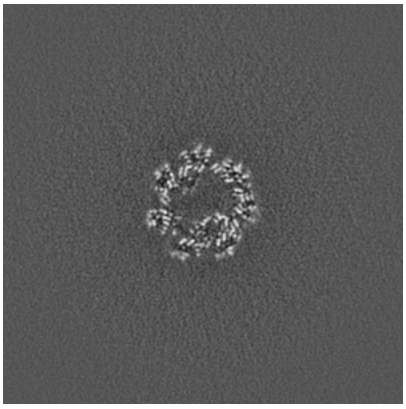
6.2.1 Primary map



X Index: 160



Y Index: 160

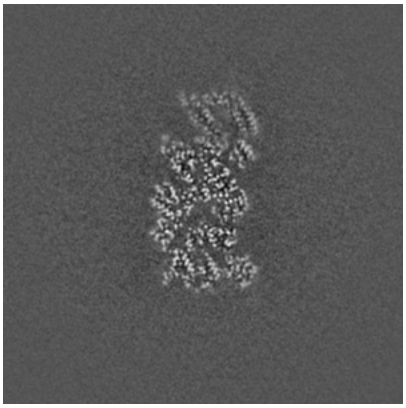


Z Index: 160

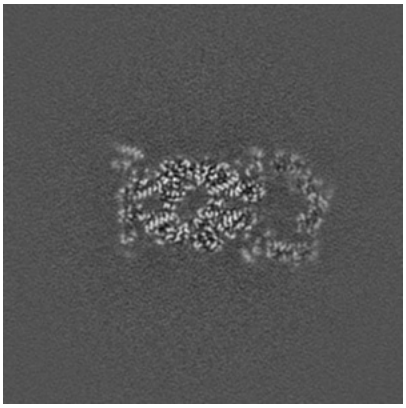
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

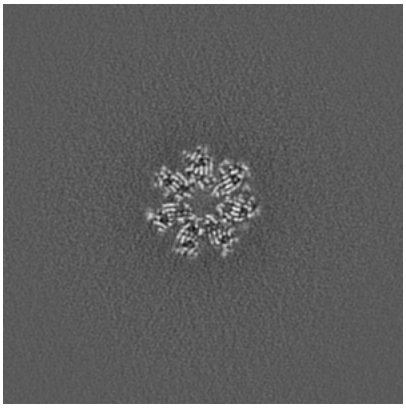
6.3.1 Primary map



X Index: 180



Y Index: 179



Z Index: 166

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

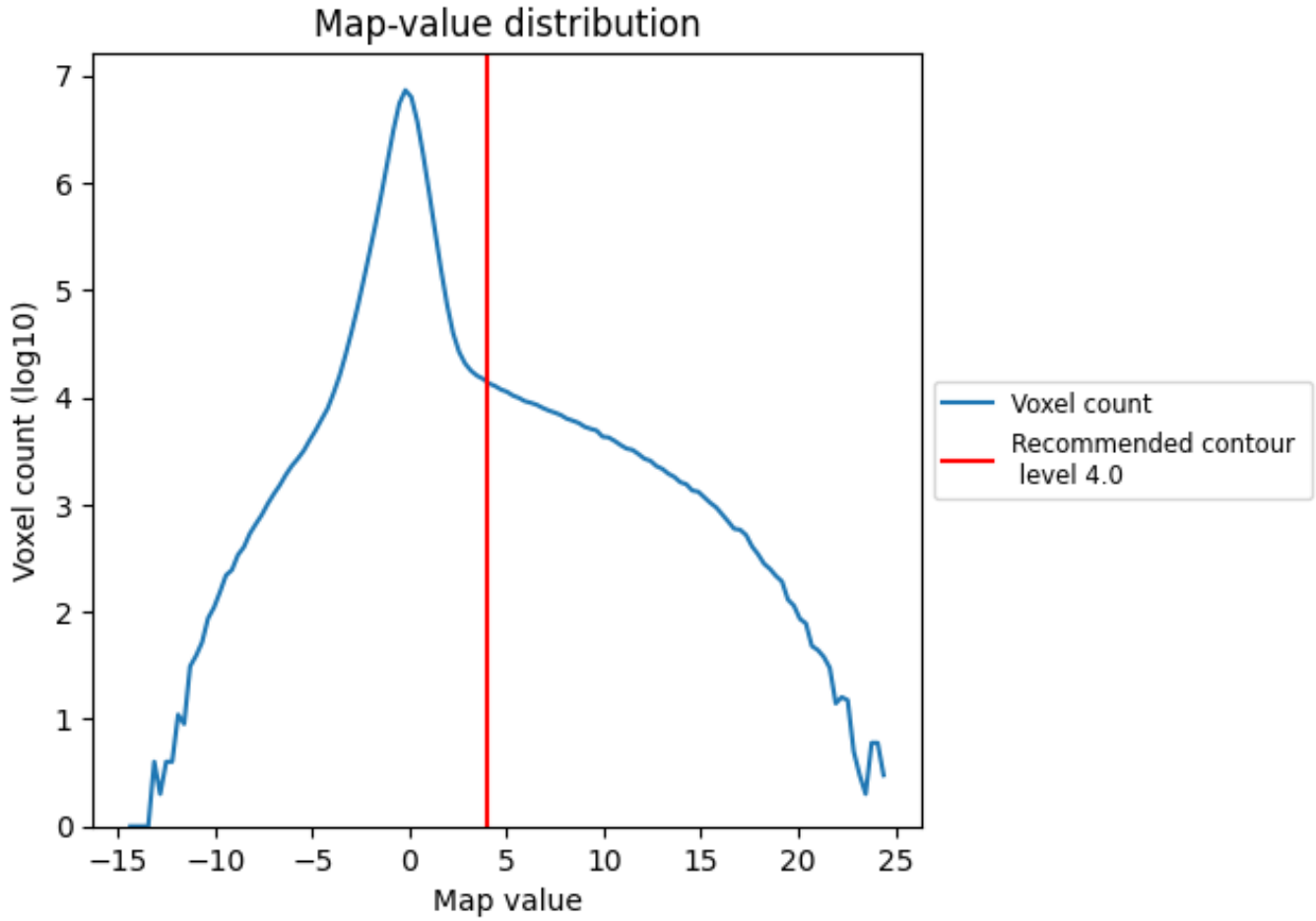
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

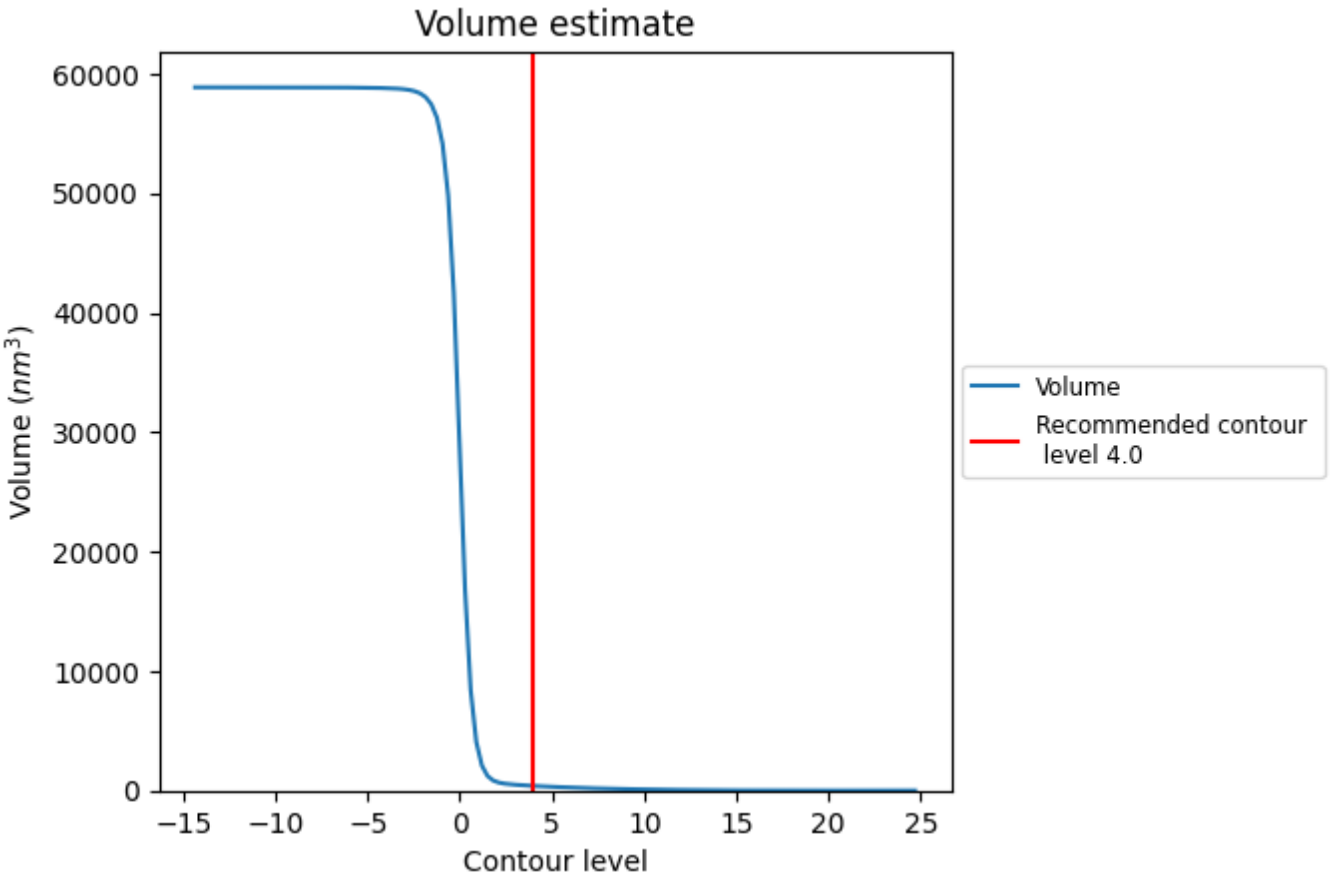
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

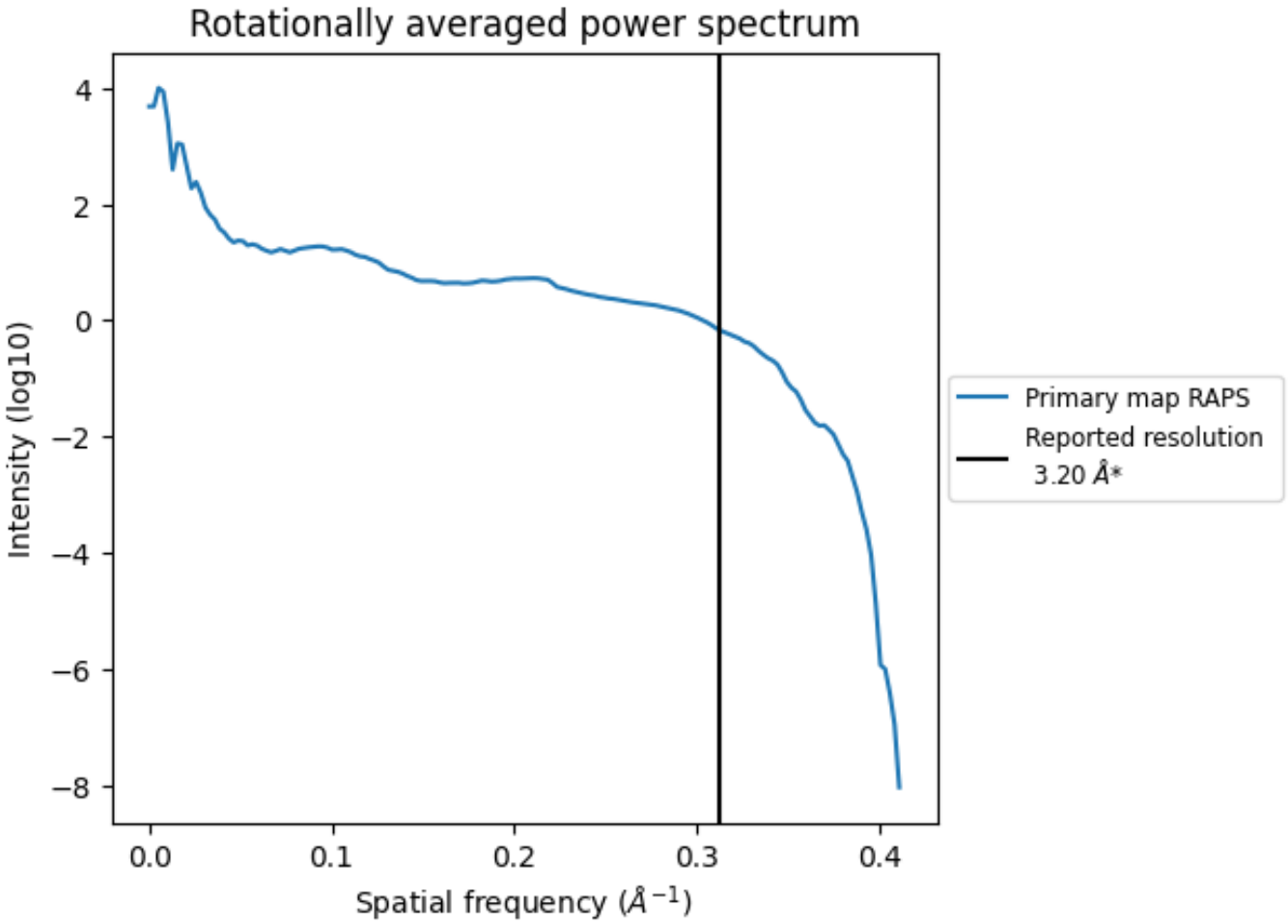
7.2 Volume estimate



The volume at the recommended contour level is 390 nm^3; this corresponds to an approximate mass of 352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

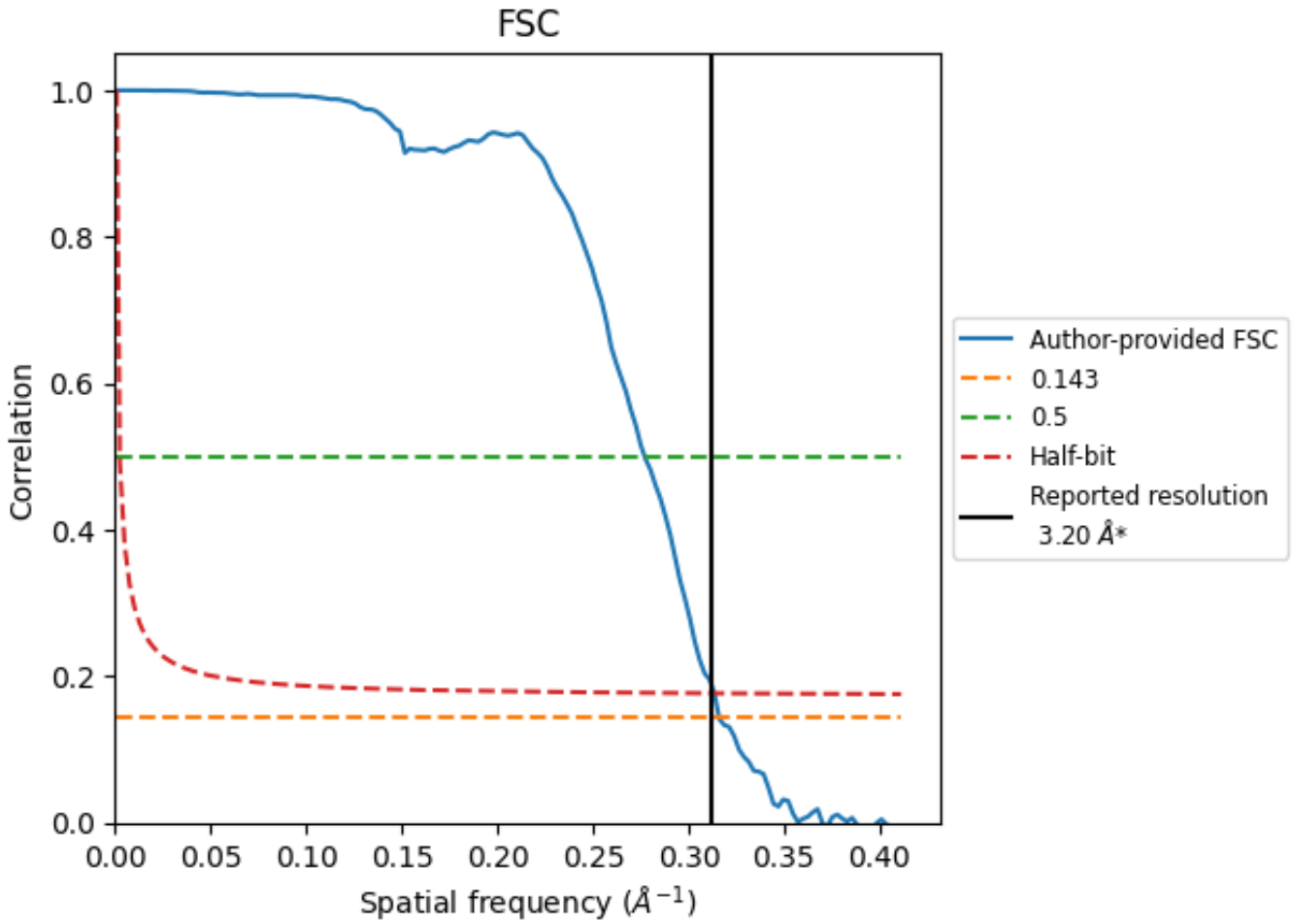


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

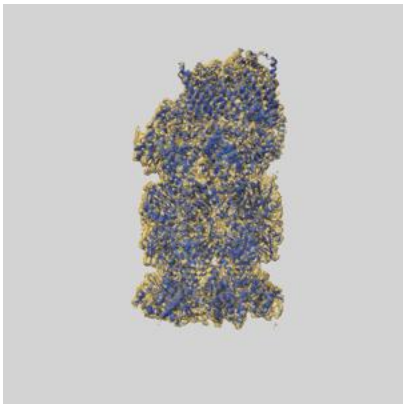
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.61	3.19
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

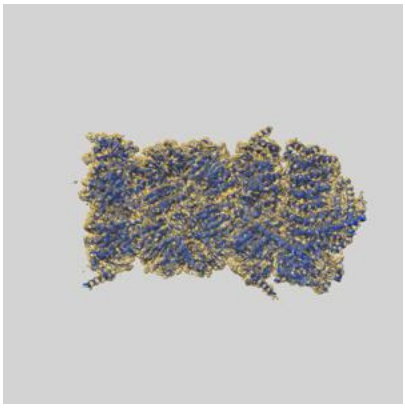
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24278 and PDB model 7NAQ. Per-residue inclusion information can be found in section 3 on page 8.

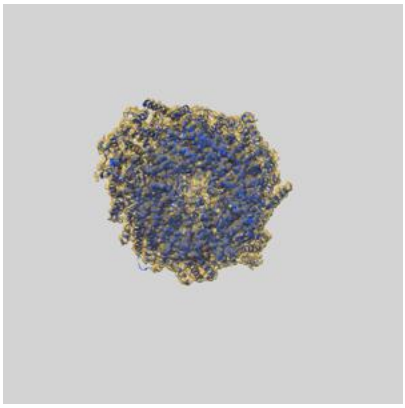
9.1 Map-model overlay



X



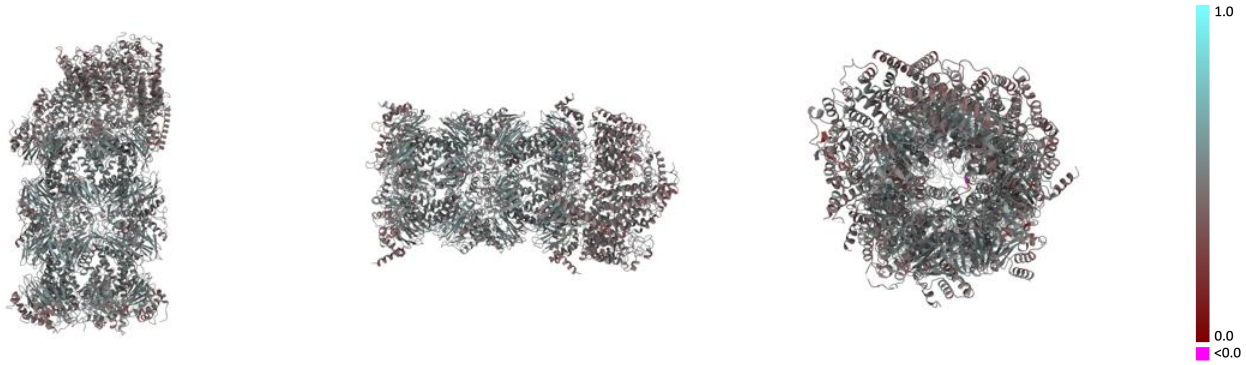
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

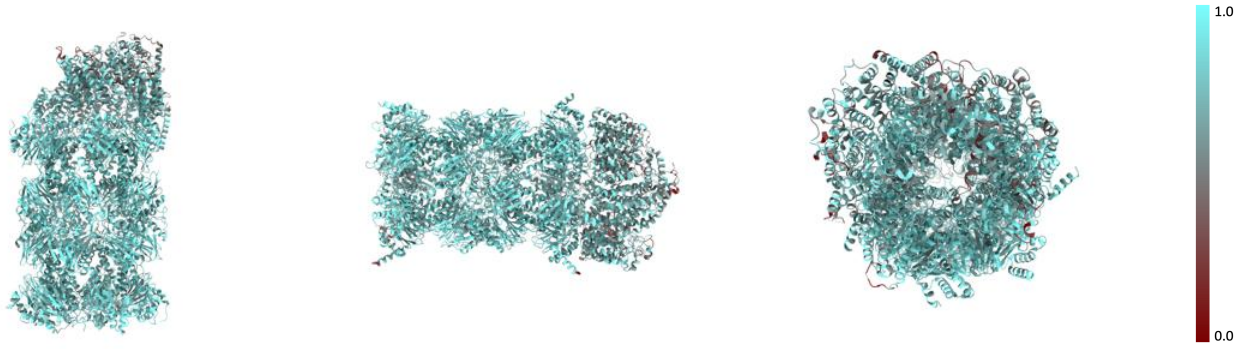
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

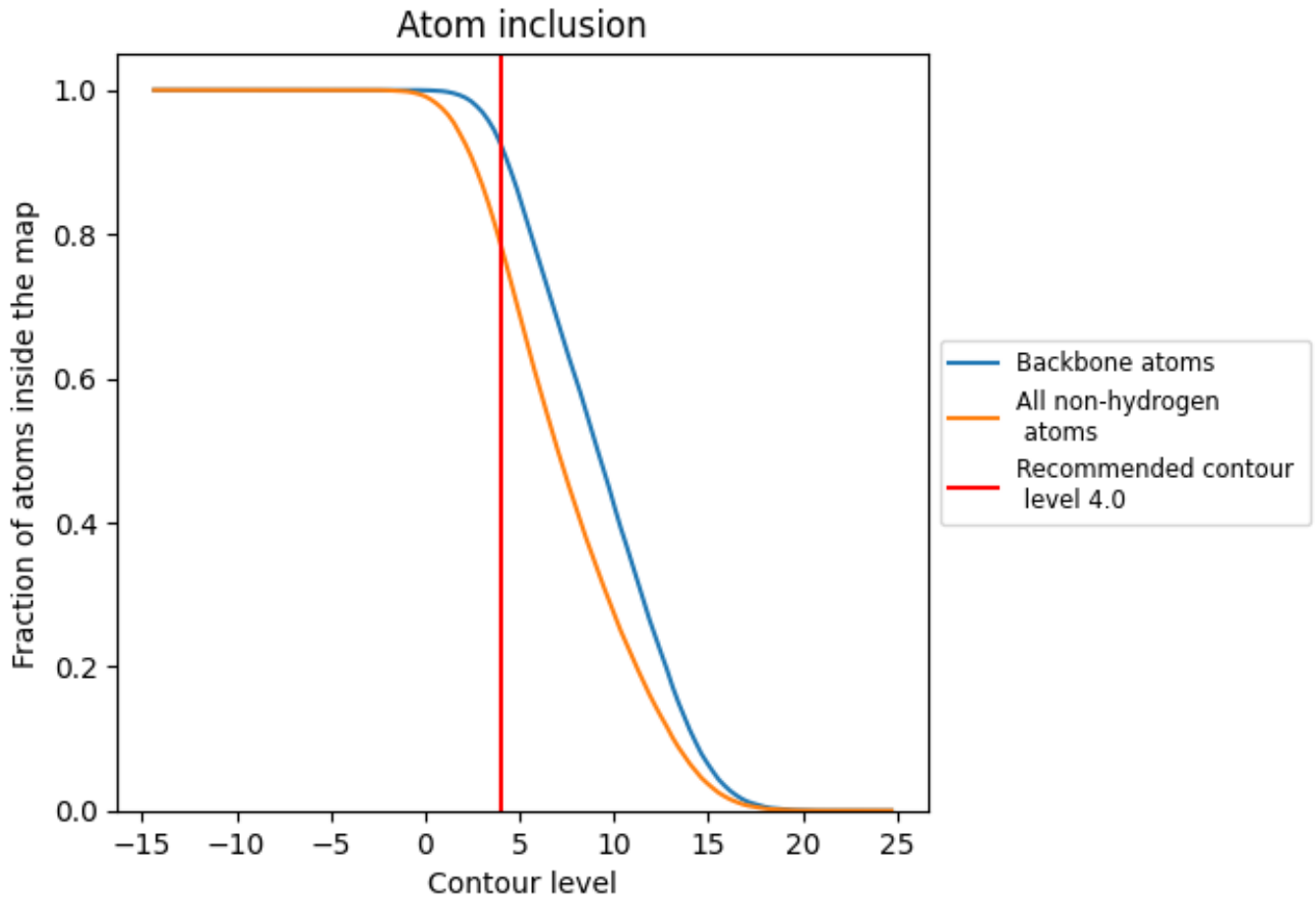
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7852	0.4830
A	0.8443	0.4950
B	0.7835	0.4770
C	0.7776	0.4650
D	0.7986	0.4840
E	0.8202	0.4890
F	0.8363	0.4920
G	0.8230	0.4900
H	0.8315	0.4990
I	0.8130	0.5090
J	0.8369	0.5110
K	0.8583	0.5050
L	0.8172	0.5040
M	0.8565	0.5120
N	0.8850	0.5200
O	0.8156	0.4900
P	0.7938	0.4780
Q	0.7965	0.4720
R	0.7708	0.4770
S	0.8181	0.4820
T	0.8106	0.4770
U	0.7909	0.4810
V	0.8171	0.4920
W	0.8239	0.5100
X	0.8391	0.5090
Y	0.8494	0.5030
Z	0.8271	0.5050
a	0.8502	0.5120
b	0.8524	0.5150
c	0.6626	0.4460